Ferromagnetism in the Hubbard model: Influence of the lattice structure

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By use of the spectral density approach the influence of the lattice structure on the possibility of ferromagnetism in the single band Hubbard model is investigated. The $d = \infty$ hypercubic lattice does not show magnetic phase transitions of second order irrespective of the strength of the Coulomb coupling. However, first order transitions to finite magnetic moments, not visible as singularities of the paramagnetic susceptibility, may appear in the very strong coupling regime. In d=3 second order transitions are found but only for very strong couplings, where the non-locality of the electronic self-energy acts in favour of the spontaneous magnetic moment. The influence of the non-local part of the self-energy is particularly strong for lattices with small coordination number. The non-bipartite fcc lattice exhibits saturated ferromagnetism for all band occupations $1 \leq n \leq 2$ while for less than half filled bands ($0 \leq n \leq 1$) the system remains in any case paramagnetic, and that for $d = 3$ as well as $d = \infty$. The Curie temperature runs through a maximum at about $n = 1.4$ and vanishes for $n \to 1$ and $n \to 2$.

I. INTRODUCTION

Originally the Hubbard model[1–3] was introduced to describe the bandmagnetism of itinerant electrons, at least qualitatively. The model Hamiltonian

$$\mathcal{H} = \sum_{i,j,\sigma}(T_{ij} - \mu)c^{\dagger}_{i\sigma}c_{j\sigma} + \frac{1}{2}U\sum_{i,\sigma} n_{i\sigma}n_{i-\sigma} \qquad (1)$$

incorporates, in the simplest way, the interplay of kinetic energy, Coulomb interaction, band structure and Pauli principle for studying magnetic and electronic properties of interacting electrons in a single non-degenerate narrow energy band. T_{ij} is the intersite hopping integral, usually taken between nearest neighbors, while U represents the Coulomb repulsion. $c_{i\sigma}$ ($c^{\dagger}_{i\sigma}$) stands for the annihilation (creation) operator of an electron with spin $\sigma =\uparrow, \downarrow$ at lattice site $\mathbf{R}_i$. By μ we denote the chemical potential. $n_{i\sigma} = c^{\dagger}_{i\sigma}c_{i\sigma}$ is the occupation number operator. The model-Hamiltonian (1) defines a non-trivial many-body problem that could be solved up to now only for some limiting cases[4–7].

Although it was soon realized, that the Hubbard model is rather a generic model for antiferromagnetism, the question whether or not the Hubbard model possesses ferromagnetic solutions continues to be the matter of controversial discussions. In this work we focus exclusively on ferromagnetic solutions of the single band Hubbard model. What concerns ferromagnetism of real substances, as Fe, Co, Ni, the direct Heisenberg exchange, Hund's rule coupling and band-degeneracy, of course, play an important role[8], the investigation of which is beyond the scope of this paper.

The Mermin-Wagner theorem[9] applied to the Hubbard model[10] excludes ferromagnetism for one- and two-dimensional lattices. For the three dimensional system with infinitely strong Coulomb repulsion ($U \to \infty$) exact results have been derived in a pioneering paper by Nagaoka[6]. For very special band fillings $n_{\pm} = (N \pm 1)/N$ (N: number of lattice sites) ferromagnetic ground states are possible; in the case of bipartite (sc and bcc) lattices for n_+ as well as for n_-, in the non-bipartite lattice (fcc) only for n_+. This indicates that the possibility of ferromagnetism crucially depends on the lattice structure. For the hypercubic (hc) lattice at infinite dimensions Fazekas et. al.[11] showed that saturated ferromagnetism is excluded. However, in a recent study Ulmke[12] applied a finite temperature Quantum Monte Carlo calculation to the Hubbard model on a fcc lattice at infinite spatial dimensions. A highly polarized ferromagnetic ground state is found in a rather wide range of band occupation. It is to be supposed that the greatest chance of ferromagnetism to appear in the single band Hubbard model is for non-bipartite lattices[13,14].

In this paper we want to investigate how sensible band ferromagnetism in the Hubbard model depends on the lattice structure, and therewith on the density of states of the non-interacting electrons (Bloch density of states: BDOS). We apply a "spectral density approach" (SDA) the reliability of which, at least for the strong coupling limit, has been demonstrated in previous papers[15–17]. The same approach has been applied to a somewhat generalized model of magnetism (multiband Hubbard model) for the band ferromagnets Fe, Co, Ni[18–20]. The SDA basically consists in a two-pole ansatz for the single-electron spectral density, justified by the rigorous moment analysis of Harris and Lange[21]. The free parameter of the ansatz are self-consistently fixed by equating exactly calculated spectral moments. The SDA turns out to be essentially equivalent to the Roth method[22,23] and to the Mori projector formalism[24,25].

For several types of BDOS we have derived the static paramagnetic susceptibility χ as a function of the band

occupation ($0 \leq n \leq 2$) and the temperature T. From the singularities we read off the instabilities with respect to ferromagnetic order. The results are confirmed by a direct calculation of the spontaneous magnetic moment. However, the χ^{-1}-zeros are due to magnetic phase transitions of second order only, while additional first order transitions to a finite spontaneous moment may occur.

The SDA statements on the possibility of ferromagnetism in the Hubbard model can be compared with recent results from the $d = \infty$-technique[12–14]. As to the lattice structure dependence the SDA solutions predict qualitatively the same trend. It is found, e.g., that for the $d = \infty$-hypercubic lattice ferromagnetism is excluded, being, on the other hand, possible for an $d = \infty$-fcc lattice.

For finite spatial dimensions ($d = 3$) we find that the non-locality of the quasiparticle self-energy, vanishing for $d \to \infty$ in the SDA, too, has a stabilizing influence on the magnetic order. As an example, the $d = \infty$ hypercubic lattice is non-magnetic, but the $d = 3$ sc lattice becomes ferromagnetic for $U/W \geq U_c/W = 4$ and $0.34 \leq n \leq 1.66$ if the full $\mathbf{k}$-dependent self-energy is taken into account. Neglecting the $\mathbf{k}$-dependent part of the self-energy drives U_c/W to a higher value ($= 14$) with n_c only slightly changed.

II. SPECTRAL DENSITY APPROACH

The method is based on a physically motivated ansatz for the single-electron spectral density, which is defined by:

$$S_{ij\sigma}(E) = \int_{-\infty}^{+\infty} dt e^{-\frac{i}{\hbar}Et} S_{ij\sigma}(t) \tag{2}$$

$$S_{ij\sigma}(t) = \frac{1}{2\pi} \langle [c_{i\sigma}(t), c^{\dagger}_{j\sigma}(0)]_+ \rangle \tag{3}$$

$[.., ..]_+$ is the anticommutator, and $\langle \ldots \rangle$ means thermodynamic averaging. The operators in (3) are thought as time-dependent Heisenberg operators. The mentioned ansatz contains some free parameters which can be fitted by equating a set of spectral moments $M^{(n)}_{ij\sigma}$

$$M^{(n)}_{ij\sigma} = \int_{-\infty}^{+\infty} dE E^n S_{ij\sigma}(E); \qquad n = 0, 1, 2, \ldots \tag{4}$$

The moments are calculated exactly via

$$M^{(n)}_{ij\sigma} = \langle \Big[\underbrace{\Big[\ldots [c_{i\sigma}, \mathcal{H}]_-, \ldots, \mathcal{H} \Big]_-}_{n\text{-fold commutator}}, c^{\dagger}_{j\sigma} \Big]_+ \rangle \tag{5}$$

In ref.[17] a two-pole ansatz for the spectral density of the strongly coupled Hubbard model is justified as a reasonable starting point requiring the fitting of the first four spectral moments. The evaluation leads to an electronic self-energy of the following structure:

$$\Sigma^{\mathrm{SDA}}_{\mathbf{k}\sigma}(E) = U\langle n_{-\sigma}\rangle \frac{E + \mu - B_{-\sigma} - F_{\mathbf{k}-\sigma}}{E + \mu - B_{-\sigma} - F_{\mathbf{k}-\sigma} - U\left(1 - \langle n_{-\sigma}\rangle\right)}. \tag{6}$$

The decisive terms are $B_{-\sigma}$ and $F_{\mathbf{k}-\sigma}$. For $B_{-\sigma} = F_{\mathbf{k}-\sigma} = 0$ (6) reproduces the Hubbard-I solution[1], which is incapable to describe ferromagnetism. $B_{-\sigma}$ as well as $F_{\mathbf{k}-\sigma}$ consists of "higher" correlation functions, possibly creating a spin-dependent shift of the Hubbard bands and therewith resulting in a finite spontaneous magnetic moment. The term $B_{-\sigma}$,

$$\langle n_{-\sigma}\rangle(1 - \langle n_{-\sigma}\rangle) B_{-\sigma} = \frac{1}{N} \sum_{i,j}^{i \neq j} T_{ij} \langle c^{\dagger}_{i-\sigma} c_{j-\sigma} (n_{i\sigma} + n_{j\sigma} - 1)\rangle, \tag{7}$$

can rigorously be expressed by the single-electron spectral density[15,17]. The other term,

$$\begin{aligned} \langle n_{-\sigma}\rangle(1 - \langle n_{-\sigma}\rangle) F_{\mathbf{k}-\sigma} = \\ \frac{1}{N} \sum_{i,j}^{i \neq j} T_{ij} e^{-i\mathbf{k}\cdot(\mathbf{R}_i - \mathbf{R}_j)} \Big[(\langle n_{i-\sigma} n_{j-\sigma}\rangle - n^2_{-\sigma}) \\ - \langle c^{\dagger}_{j\sigma} c^{\dagger}_{j-\sigma} c_{i-\sigma} c_{i\sigma}\rangle - \langle c^{\dagger}_{j\sigma} c^{\dagger}_{i-\sigma} c_{j-\sigma} c_{i\sigma}\rangle \Big], \end{aligned} \tag{8}$$

incorporates a density-density, a double hopping-, and a spinflip-correlation. For the evaluation of these expectation values properly modified spectral densities,

$$S^{(A)}_{ij\sigma}(t) = \frac{1}{2\pi} \langle [A_i(t), c^{\dagger}_{j\sigma}(0)]_+ \rangle, \tag{9}$$

are introduced, where the operator A_i is chosen in such a way that the respective expectation value can be derived directly via the spectral theorem from $S^{(A)}_{ij\sigma}(E)$. It can be justified by inspection of the Lehmann representation of these functions that in the wave-vector representation they must represent two-pole functions as the original single-electron spectral density (2). The various functions (2) and (9) differ only by the spectral weights of the poles. For fixing $S^{(A)}_{ij\sigma}(E)$ one therefore needs only two respective moments. Doing so one finally arrives at a closed system of equations that can be solved self-consistently for all quantities of interest. For further details the reader is referred to[17].

We study the magnetic phase transition by use of the static susceptibility

$$\chi(T, H, n) = \frac{1}{\mu_0} \left(\frac{\partial M}{\partial H} \right)_{T,n}. \tag{10}$$

μ_0 is the vacuum permeability and H a homogeneous static magnetic field. M denotes the magnetization

$$M = \frac{N}{V}\mu_B(\langle n_\uparrow\rangle - \langle n_\downarrow\rangle). \qquad (11)$$

We calculate χ for the paramagnetic system in the zero-field limit. The poles of the susceptibility indicate the instabilities of the system towards ferromagnetic ordering. To calculate the static susceptibility χ we have to include a Zeeman term in the Hamiltonian (1). When differentiating M with respect to the external field one has to bear in mind that all expectation values $\langle \ldots \rangle$ are field-dependent.

III. RESULTS

We have investigated the tendency to ferromagnetism in the single band Hubbard model for several lattice structures and different spatial dimensions. The zeros of the inverse static paramagnetic susceptibility indicate the magnetic phase transitions of second order. Fig. 1 shows the results for a sc lattice.

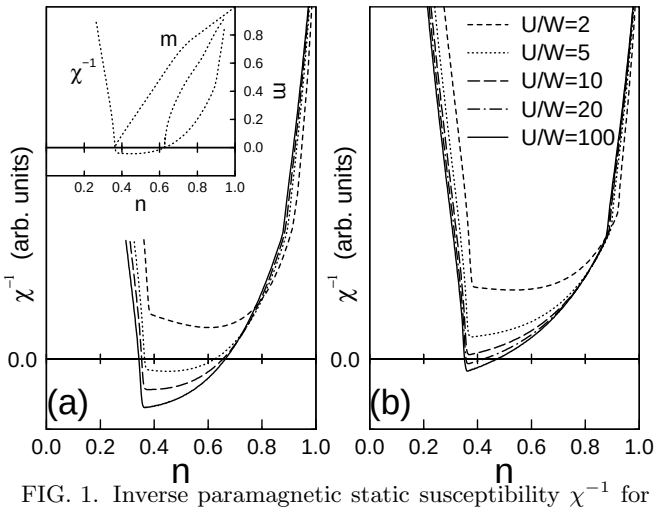

FIG. 1. Inverse paramagnetic static susceptibility χ^{-1} for the sc lattice ($d = 3$) as a function of the band occupation n for various values of the Coulomb interaction U. (a) System with the full $\mathbf{k}$-dependent self-energy. (b) System with a local self-energy ($F_{\mathbf{k}-\sigma} \equiv 0$ artificially, see eq. (6)). The inset in (a) shows the magnetization curves $m(n)$ of the two ferromagnetic solutions starting at the two zeros of χ^{-1} for $U/W = 5$. ($T = 0\,\mathrm{K}$).

Sometimes it is argued[26] that for this bipartite lattice ferromagnetism is hardly to be expected. On the other hand, Shastry et. al.[27] report for the $d = 3$ model even saturated ferromagnetism for $n \geq 0.68$. That is very close to our findings. It is a special feature of the SDA[15–17], possibly even for the Hubbard model itself, that there are two ferromagnetic solutions, i. e. two zeros of χ^{-1}. The first solution sets in at $n_c^{(1)} = 0.34$ ($U \to \infty$), where the actual value only slightly depends on U. This solution runs into saturation for $n \geq 0.68$ ($U \to \infty$), in exact agreement with the results of ref.[27]. The second solution appears for higher band occupations, but does never reach saturation. This less magnetized solution is always less stable and can be disregarded in the following discussion. In spite of the appearance of ferromagnetic solutions the sc structure seems not to be very convenient for a spontaneous order. A rather strong Coulomb coupling $U/W > 4$ (W: Bloch bandwidth) is needed. In this context it is interesting to look at the influence of the non-locality of the electronic self-energy (6). The wave-vector dependence comes into play due to the higher correlation functions in $F_{\mathbf{k}-\sigma}$ (8). Since in the limit of infinite spatial dimensions the electronic self-energy is wave-vector independent[28], the role of the $\mathbf{k}$-dependent terms in $\Sigma^{\mathrm{SDA}}_{\mathbf{k}\sigma}(E)$ might be underestimated for $d = 3$. In part (b) of Fig. 1 we have plotted χ^{-1} as function of the electron density for the case that the self-energy (6) has been made local simply by setting $F_{\mathbf{k}-\sigma} \equiv 0$. The critical couplings U_c/W for ferromagnetic order rises enormously from 4 for the full $\mathbf{k}$-dependent self-energy (Fig. 1(a)) to 14 for the local self-energy (Fig. 1(b)). Its influence on magnetic stability, however, is not for all cubic lattices of the same importance. It can be recognized that with increasing number of nearest neighbours the importance of the $\mathbf{k}$-dependent part of the self-energy rapidly decreases. For the fcc lattice ($Z_1 = 12$) it appears already non-remarkably[16].

In infinite spatial dimensions, for which the higher correlation $F_{\mathbf{k}-\sigma}$ disappears, we do not find zeros in χ^{-1} for the hypercubic lattice (inset of Fig. 2), and that irrespective of the strength of the Coulomb coupling U. Phase transitions of second order are therefore excluded.

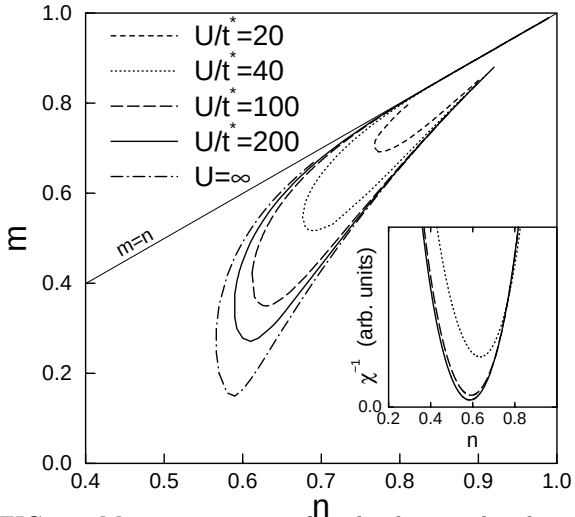

FIG. 2. Magnetization m for the hypercubic lattice in $d = \infty$ as a function of the band occupation n for various values of the Coulomb interaction U. The BDOS is given by: $\rho_0(E) = \exp(-0.5(E/t^*)^2)/(t^*\sqrt{2\pi})$. Inset: Inverse paramagnetic static susceptibility χ^{-1} as a function of the band occupation n. ($T = 0\,\mathrm{K}$).

The same fact has been reported by Jarrell[29] who elaborated a self-consistent Monte Carlo procedure, which is claimed to be essentially exact for the $d = \infty$ Hubbard model. Although there is no indication for ferromagnetism in the static susceptibility, the direct evaluation of the SDA for the spin-dependent, averaged particle numbers $\langle n_\uparrow \rangle$, $\langle n_\downarrow \rangle$ reveals ferromagnetic solutions (Fig. 2). They belong to first order transitions being therefore not visible as χ^{-1}-zeros. These solutions appear for rather strong Coulomb couplings and for band occupations $n \geq 0.57$. For a given U the $m(n)$ curve forms a closed bubble steadily contracting itself for increasing temperature. For a given band occupation n this means a first order transition at a certain critical temperature. Ferromagnetic saturation is, strictly speaking, never reached, not even for $T = 0K$ (Fig. 2). This is because of the infinite tails of the Gaussian BDOS. The strict physical meaning of this kind of ferromagnetism in the Hubbard model requires further investigation.

It turns out that the three dimensional bcc lattice with its divergence at the center of the BDOS is much more convenient for ferromagnetism than the sc lattice. Already for $U/W \approx 1$ two ferromagnetic solutions appear, the stable one starts for $U \to \infty$ at $n_c = 0.52$ reaching saturation (m=n) for $n \geq 0.68$ (Fig. 3).

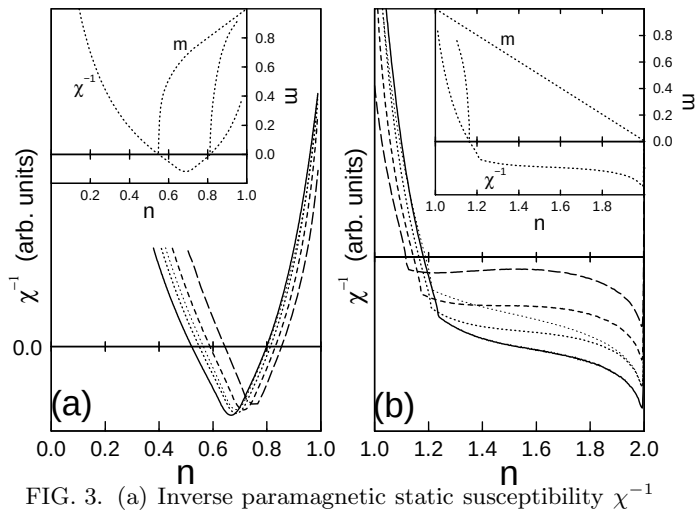

FIG. 3. (a) Inverse paramagnetic static susceptibility χ^{-1} for the bcc lattice as a function of the band occupation n for various values of the Coulomb interaction U (parameters as in Fig. 1(b)). The thin dotted line corresponds to the system with the local self-energy ($F_{\mathbf{k}-\sigma} \equiv 0$ artificially, see eq. (6)) for $U/W = 5$. The inset shows the magnetization curves $m(n)$ together with χ^{-1} for $U/W = 5$. (b) the same as in (a) for the fcc lattice. ($T = 0\,\mathrm{K}$).

The latter result is again in exact agreement with the findings in ref.[27], where the stability of the Nagaoka state[6] ($U/W \to \infty$) with respect to an electron spin flip is investigated. As already mentioned the **k**-dependence of the electronic self-energy has not such dramatic consequences as for the sc lattice (Fig. 1).

The non-bipartite fcc lattice does not allow ferromagnetism for less than half-filled energy bands. However, for the more than half-filled band we find saturated ferromagnetism ($m = 2 - n$: "Nagaoka state") for all electron densities $1.0 \leq n \leq 2.0$ indicated by a zero of χ^{-1} at $n = 2.0$ (Fig. 3). This agrees with the investigation of Müller-Hartmann et. al.[13] who employed the single spin flip Gutzwiller variational states of Shastry et. al.[27] and corrected their value of $n_c = 1.62$ in[27] to $n_c = 2.0$. For electron densities $1.0 \leq n \leq 1.2$ the SDA yields a second ferromagnetic solution which is less stable than the fully polarized one.

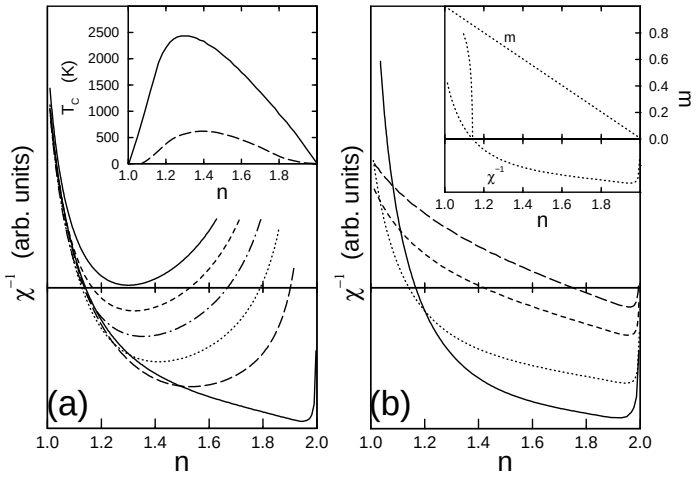

FIG. 4. fcc lattice in $d = \infty$ (BDOS: $\rho_0(E) = \exp(-0.5(1+\sqrt{2}E))/\sqrt{\pi(1+\sqrt{2}E)}$ from ref.[12]) (a) Inverse paramagnetic static susceptibility $\chi^{-1}(n)$ as a function of the band occupation n for various temperatures T (solid: $T = 0\,\mathrm{K}$, long dashed: $T = 500\,\mathrm{K}$, dotted: $T = 1000\,\mathrm{K}$, dot dashed: $T = 1500\,\mathrm{K}$, dashed: $T = 2000\,\mathrm{K}$, dot dot dashed: $T = 2500\,\mathrm{K}$.) The inset shows the Curie temperature T_C as a function of the n. The solid line is the result of the SDA, the long dashed line is taken from ref.[12]. ($U = 4\,\mathrm{eV}$). (b) $\chi^{-1}(n)$ for various values of the Coulomb interaction U. The inset shows the magnetization curves $m(n)$ together with χ^{-1} for $U = 4\,\mathrm{eV}$. (long dashed: $U = 0.4\,\mathrm{eV}$, dashed: $U = 1\,\mathrm{eV}$, dotted: $U = 4\,\mathrm{eV}$, solid: $U = 100\,\mathrm{eV}$; $T = 0\,\mathrm{K}$).

The results are qualitatively similar for the Hubbard model on the infinite dimensional fcc lattice (Fig. 4). Here, we used the BDOS given in ref.[12]. The $\chi^{-1}(n)$ curves exhibit two zeros due to two ferromagnetic solutions as in the $d = 3$ case (Fig. 3). The fully polarized state ($m = 2 - n$) is stable for all band occupations $1.0 \leq n \leq 2.0$ with a critical coupling $U_c(n = 2.0)/W = 0^+$. The same is reported in ref.[12,14]. The asymmetric BDOS of the non-bipartite fcc lattice is obviously very convenient for the band ferromagnetism in the more than half filled single band Hubbard model.

For finite temperature the χ^{-1}-zero shifts away from $n = 2.0$ to lower values indicating a Curie-temperature of $T_C = 0^+$ for $n = 2$ (Fig. 4(a)). The $T_C(n)$ curve runs through a maximum at $n \approx 1.4$ and goes to zero for the half-filled ($n \to 1.0$) and the fully occupied ($n \to 2.0$) energy band (see inset in Fig. 4(a)). These results are qualitatively consistent with that of Ulmke[12]. However, contrary to ref.[12], our $T_C(n)$ curve persists until $n = 1$. This reflects the fact, that close to half filling ($1.0 < n < 1.15$) the magnetization curves in the SDA exhibit first order phase transitions as a function of temperature. Magnetic solution of this kind where not considered in ref.[12]. Quantitatively our T_C-values are on an average higher by a factor 4, but nevertheless in a reasonable order of magnitude.

IV. CONCLUSIONS

By use of a spectral density approach we have demonstrated the striking influence of the lattice structure on the possibility of ferromagnetism in the Hubbard model. The zeros of the inverse static paramagnetic susceptibility indicate the onset of ferromagnetic order in dependence of typical variables as the band occupation n and temperature T. In the hc lattice no "normal" ferromagnetism appears at infinite dimensions, while for $d = 3$ (sc lattice) magnetic solutions are found if U/W exceeds a rather high critical value. For small lattice coordination number (e.g. sc lattice) the non-locality of the electronic self-energy favours ferromagnetism in a remarkable manner. In the non-bipartite fcc lattice no magnetism exists for less than half-filled bands, while for $1.0 \leq n \leq 2.0$ saturated ferromagnetism is found at $d = 3$ as well as $d = \infty$.

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